above and in the figures are hereby incorporated by reference in their entirety. Walker et al., *Nature*, 402:313-320, is incorporated by reference in its entirety, including Figs. 1-7.

Table 1 Data collection, structure determination and refinement statistics

Data collection and multiple isomorphous replacement phasing statistics

Data set	Resolution (Å)	Observations/ unique reflections	Completeness (last shell) (%)	R_{merge}‡‡	$\langle I/\sigma \rangle$ (last shell)	No. of sites	Phasing power‖‖	R_{iso}§§
Native*††	2.4	144,973/37,485	97 2 (90.6)	8.5	16.0 (3 1)	–	–	–
$LuCl_3$-1†*	2.2	191,292/49,599	95.5 (93 3)	9.5	14.3 (1.1)	7	1.7	0 23
$LuCl_3$-2‡††	3 5	43,038/12,484	99.7 (98 2)	8 5	11.3 (3.4)	3	1 9	0 18
Lanthanides§††	3 0	71,426/19,180	97.9 (97.1)	4 5	15 6 (2.3)	8	1 9	0 24
ATM‖††	2 7	94,900/25,688	92 6 (60 2)	4 8	17 0 (5 7)	5	0 8	0 22
Iodine¶††	2 6	102,511/28,856	93 2 (67.1)	6 0	13 6 (1 4)	3	0 1	0 21

Refinement statistics #

Data set	Resolution (Å)	Protein atoms	Waters	$R_{crystal}$¶¶	R_{free}¶¶ (% data)	R.m.s.d. from ideality##		
						Bonds	Angles	Dihedrals
$LuCl_3$-1	25.0–2 2	6,813	89	0 25	0 30 (5.4)	0.013 Å	1 7°	23°
Iodine¶	25 0–2 6	6,954	14	0 26	0.33 (5.0)	0.005 Å	1 1°	21°
Mn#	25.0–2.6	6,837	26	0 26	0.32 (5.6)	0.005 Å	1 2°	21°

Overall figure of merit 0 45

* The native crystal was soaked in 2 5 mM $InsP_3$, 1.0 mM ATP and 10 mM $MgCl_2$ for 1 h. Although this was the native crystal for heavy-atom phasing, the final high-resolution structure refinement used data from $LuCl_3$-1.

† $LuCl_3$-1 crystal was soaked in 20 mM $LuCl_3$ and 1.25 mM ATP for 1 h 40 min.

‡ $LuCl_3$-2 crystal was soaked in 20 mM $LuCl_3$ and 1.3 mM ATP for 4 h.

§ Lanthanides crystal was soaked for 4 h in a mixture of 3.3 mM each of $GdCl_3$, $TbCl_3$, $HoCl_3$, $ErCl_3$, $TmCl_3$, and $LuCl_3$ with 1 26 mM ATP and 1 mM EMTS.

‖ ATM crystal was soaked for 22 h in 10 mM sodium aurothiomalate.

¶ Iodine crystal was soaked for 75 min in 1 mM NaI_3 and 1 mM chloramine T. This crystal was originally prepared in an attempt to iodinate tyrosine residues as a heavy atom derivative, but no evidence of tyrosine iodination was seen in the resulting structure.

Mn crystal contained 1.4 mM ATP and 14 mM $MnCl_2$.

* Data were collected at ESRF beamline ID2b.

†† Data were collected at ESRF beamline ID14-4.

‡‡ $R_{merge} = \Sigma_{hkl}\Sigma_i|I_i(hkl) - \langle I(hkl)\rangle|/\Sigma_{hkl}\Sigma_i I_i(hkl)$.

§§ $R_{iso} = \Sigma||F_{deriv}| - |F_{native}||/\Sigma|F_{native}|$.

‖‖ The phasing power is defined as the ratio of the r.m.s. value of the heavy atom structure factor amplitudes and the r.m.s. value of the lack-of-closure error.

¶¶ R_{cryst} and $R_{free} = \Sigma|F_{obs} - F_{calc}|/\Sigma F_{obs}$; R_{free} calculated with the percentage of the data shown in parentheses.

R.m.s. deviations for bond angles and lengths in regard to Engh and Huber parameters.